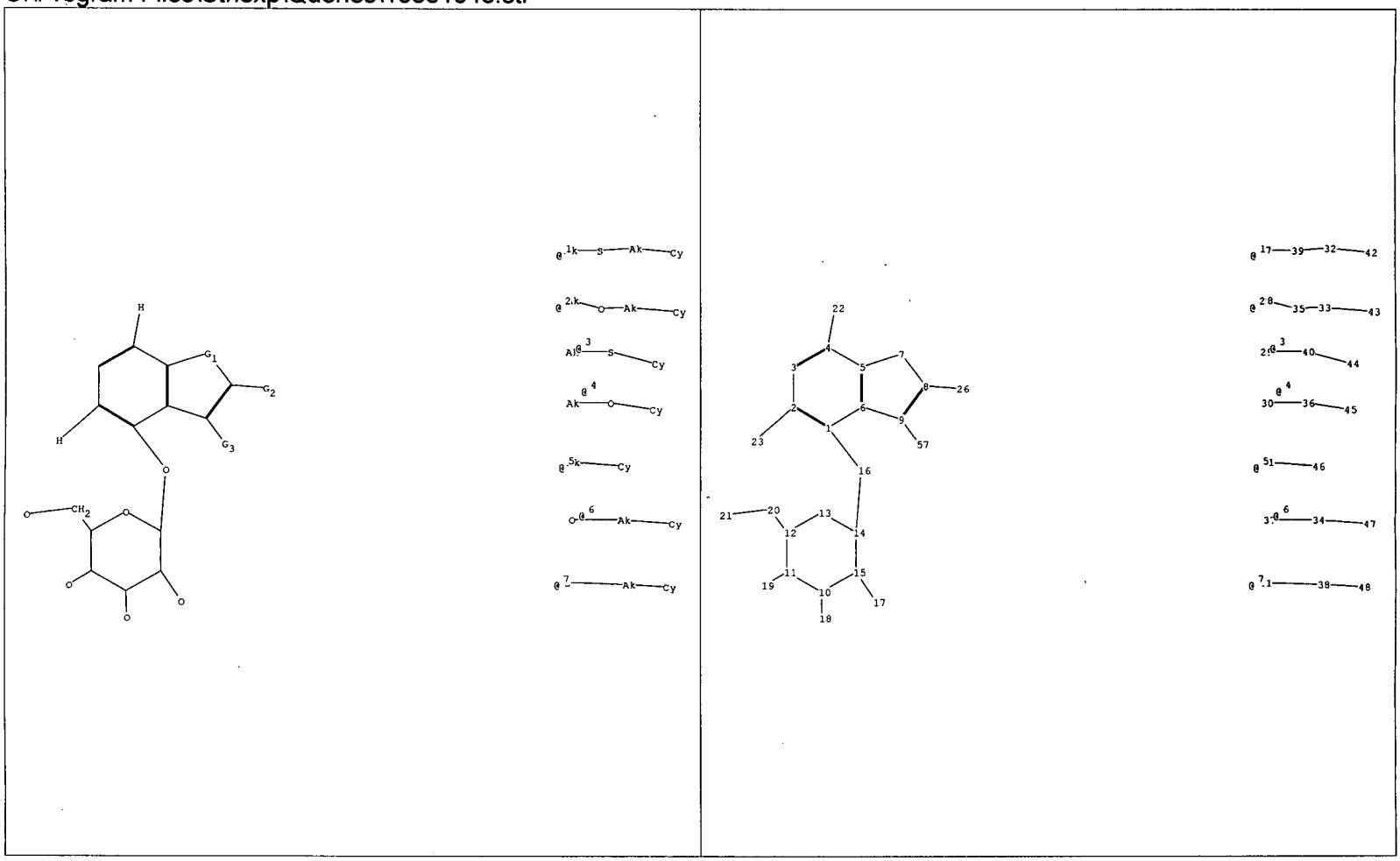
C:\Program Files\Stnexp\Queries\10551648.str



chain nodes :
16 17 18 19 20 21 22 23 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 57
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
1-16 2-23 4-22 8-26 9-57 10-18 11-19 12-20 14-16 15-17 20-21 27-39 28-35 29-40 30-36 31-46 32-39 32-42 33-35 33-43 34-37 34-47 36-45 38-41 38-48 40-44
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-16 2-23 4-22 5-7 6-9 7-8 8-9 8-26 9-57 10-11 10-15 10-18 11-12 11-19 12-13 12-20 13-14 14-15 14-16 15-17 20-21 27-39 28-35 29-40 30-36 31-46 32-39 32-42 33-35 33-43 34-37 34-47 36-45 38-41 38-48 40-44
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S,N

G2:H,X,Ak

G3:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS